The phonon Spectrum, Phonon-Phonon Interaction and Infrared Dielectric Response from First Principles

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Abstract

We present our first-principles algorithms for calculating phonon spectra and the infrared dielectric response. The harmonic approximation, phenomena exhibited by polar crystals, and the relevance of anharmonic effects to optical properties are reviewed. Lattice dynamics are treated within a frozen-phonon formalism incorporating the theory of macroscopic polarization. Modern developments in the theories of dielectric polarization and the phonon-phonon interaction are essential elements to our detailed spectral analysis of the infrared dielectric function. The results of our study of GaAs are compared to measurement.

The work is done in close collaboration with Hadley M. Lawler (University of Maryland) and Eric K. Chang (Univeristy of Modena).